



## Interagency Coordinating Committee on the Validation of Alternative Methods

# Data Sharing

Nicole C. Kleinstreuer, PhD  
NICEATM Deputy Director

SACATM Meeting

September 18-19, 2017

Agency for Toxic Substances and Disease Registry • Consumer Product Safety Commission • Department of Agriculture  
Department of Defense • Department of Energy • Department of the Interior • Department of Transportation  
Environmental Protection Agency • Food and Drug Administration • National Institute for Occupational Safety and Health  
National Institutes of Health • National Cancer Institute • National Institute of Environmental Health Sciences  
National Library of Medicine • Occupational Safety and Health Administration



## **Strategic Goal: Foster the use of efficient, flexible, and robust practices to establish confidence in new methods**

- Identify and collate sources of high-quality human toxicological data.
- Create centralized data access points that are publicly available and easily accessible.
- Actively solicit the submission and collation of parallel data from animal studies and alternative methods.
- Leverage partnerships and complimentary initiatives
  - FAIR Principles, Biomed21 recommendations, SEND reporting, NIH Data Commons, NCATS Data Translator, EPA Chemistry Dashboard, NLM Databases, etc.



## FAIR PRINCIPLES

<b>Findable</b>	A data object should be uniquely and persistently identifiable.
<b>Accessible</b>	Data is accessible by authorized users (human and machine) through a well-defined protocol.
<b>Interoperable</b>	(Meta) data assigned to the data object is syntactically parse-able and semantically machine accessible.
<b>Reusable</b>	Data objects must comply with the above three principles and sufficiently documented to allow integration/linkage with other data sources.

<https://www.force11.org/fairprinciples>

*Wilkinson et al. 2016*



## State of FAIRness at NIEHS

- Microcosm of larger research enterprise
- Heterogenous mix of:
  - Data systems and technologies
  - Data management practices
  - Metadata capture and standards
  - Funding mechanisms for building & sustaining systems
  - Teams and talent around building & maintaining systems
  - Policies around usage of data
- Common data publication practices in place:
  - submission to *dbGAP*, *GEO*, *clinicaltrials.gov*, ...





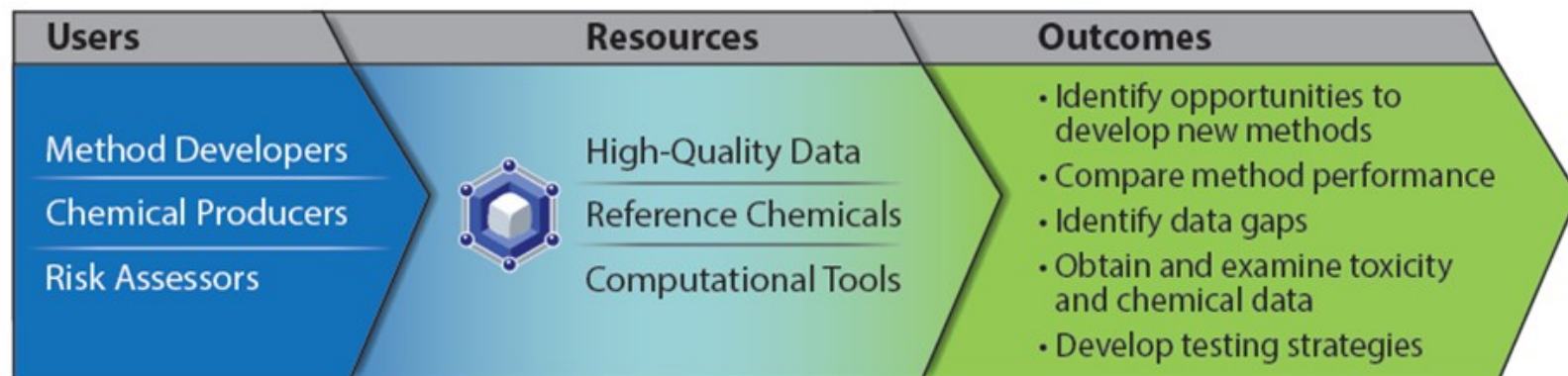
## State of FAIRness at NICEATM

- **Integrated Chemical Environment (ICE)**

- <https://ice.ntp.niehs.nih.gov/>



- Provides FAIR for ICCVAM data
- Feeder into other applications and data systems
  - Chemical Effects in Biological Systems (CEBS)
  - CTD, EPA databases, etc.
- Significant ongoing efforts to improve data utility
  - Intuitive user interface
  - Web-based visual analytics
  - Improved search functionality
  - Improving capture of data provenance
  - Web application programming interfaces (APIs)
  - Many more...



<https://ice.ntp.niehs.nih.gov/>

- Integrated Chemical Environment: ICE
  - Structured format designed for ease of use
  - Allows access to data for multiple regulatory endpoints
  - Query by CASRN or established reference chemical lists
  - Flexible, exportable results
    - Both in computer-friendly format and a human-friendly summary format for quickly comparing data between chemicals



## Interagency Coordinating Committee on the Validation of Alternative Methods

Secure | <https://ice.ntp.niehs.nih.gov/#!Search>



Integrated  
Chemical  
Environment

Home

Integrator

Workflows

Reference Data

About ▾

Help ▾

Run Search

Clear

Select Assays

Union ▾



[View Data Sets](#)

Select Assay Target

Activity

☒ Acute Oral Toxicity

☒ Skin Sensitization

Any ▾

☒ Skin Irritation

Any ▾

☒ Eye Irritation

Any ▾

☒ Endocrine

Any ▾

☒ in vitro (all)

Any ▾

☒ in silico

Any ▾

Select Chemicals



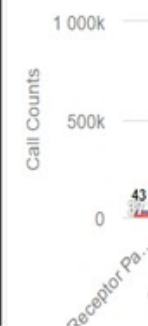
Download



Number of chemicals = 43877. Showing 20 out of 60 Endpoints. All Endpoint columns are exportable.

Substance Name	CASRN	Acute Oral Toxicity...	Acute Oral Toxicity...	DPRA Depletion L...	DPRA Ca
Acetamide	60-35-5				
Acetaminophen	103-90-2	2404	[0.32-3.43], n=2, ...		
Acetohexamide	968-81-0				
Acetonitrile	75-05-8				
Dehydroacetic acid	520-45-6				
1-Acetyl-2-phenyl...	114-83-0				

### Chemical Breakdown



<https://ice.ntp.niehs.nih.gov/>



## Challenges facing FAIR

- IR (interoperable, reusable) are especially challenging
  - Depends on the questions being asked
  - Requires agreement and coordination across parties
- Not all data can be moved
  - Issues based on policy, size
  - Computation must be moved to the data
- Finite resources
  - Community must guide what data and type of access is prioritized





## BioMed21 (26-27 June 2017)

<http://www.biomed21.org>

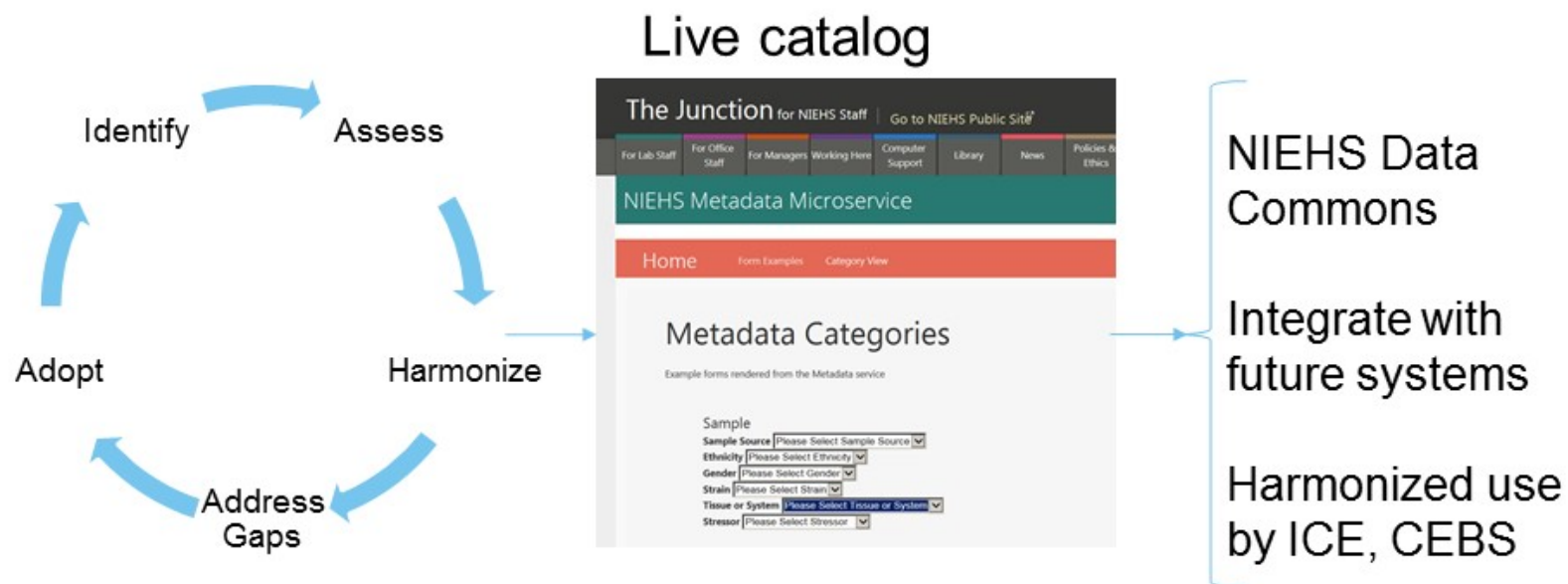
- Standardization of data reporting (e.g. SEND)
- Data availability and accessibility
- Data quality and relevance
- Ontological classification and data integration
- Multi-layer communication protocols
- Systems biology approaches
- Establishing partnerships



## BioMed21: Major Recommendations

- International and inter-agency collaboration is critical: formal collaboration between major organizational and funding bodies should be established
- Funding should be prioritized for researching human-based biology and promoting open access data
- Human data should be collected in collaborative, open-access high-quality databases
- Common reporting formats and common ontologies should be established for collecting and collating human biology information, from different 'omics technologies to human clinical data
- There is a need to establish formal processes for cross-sector communication
- There is an immediate need for the creation of case studies to demonstrate applications and benefits of predictive, mechanism-based approaches

# Towards Common Terminology



*Effort being led by Charles Schmitt, NIEHS/ODS*



## Evaluating Data Quality

- Understanding reproducibility, relevance, and readability
- Establishing minimum criteria for animal study data based on guideline protocols
  - Ex: Uterotrophic database (*Kleinstreuer et al. 2016*)
- Semi-automated retrieval and evaluation of published literature
  - Project with Oak Ridge National Labs (ORNL) to apply text-mining approaches to identify high-quality data





# Interoperability Across Systems

Consistent & compatible web-APIs



CEBS



ICE

Others...



Data Commons

NIEHS Data Systems

Consistent data set access & retrieval



CSS Dashboard

PubChem

Many others...



External Data Systems





## Acknowledgments

- NICEATM staff
- ICCVAM members
- BioMed21 participants
- NIEHS DNTP
  - Mary Wolfe, John Bucher, Andy Shapiro
- NIEHS Office of Data Science
  - **Charles Schmitt**, Stephanie Holmgren